# Transport Methods for the CAM Spectral Element Dynamical Core

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MS17 Numerical Methods for the Ocean and Atmosphere

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# Motivation

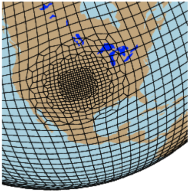
*Why are transport schemes so important?*

- Atmosphere is the most expensive component of CESM
- Tracer advection is 50% of total cost for 26 tracers
- With biogeochemistry 100-1000 tracers are needed

**ACES4BGC**
Applying Computationally Efficient Schemes for BioGeochemical Cycles

*Objective:*

- Implement and optimize new computationally efficent tracer advection algorithms for large numbers of tracer species that
  - work on fully unstructured grids
  - exploit the fact that we will be transporting hundreds of species



# Transport Problem

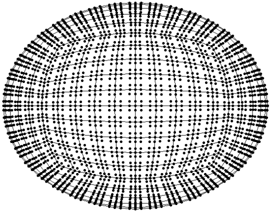
*A tracer, represented by its mixing ratio $q$ and mass $\rho q$, is transported in the flow with velocity $\mathbf{u}$*

$$\left.\begin{array}{l} \dfrac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \\[2ex] \dfrac{\partial \rho q}{\partial t} + \nabla \cdot \rho q \mathbf{u} = 0 \end{array}\right\} \rightarrow \frac{Dq}{Dt} = 0$$

*Solution methods should satisfy*

- local conservation of $\rho q$
- monotonicity or bounds preservation of $q$
- consistency between $q$ and $\rho$ (free stream preserving)

# Spectral Element Dynamical Core



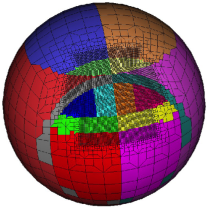
- Continuous Galerkin finite element method using Gauss-Lobatto quadrature
- Generally runs on the cubed sphere grid, but applicable to any unstructured quadrilateral grid on the sphere

Advection using the standard spectral element method with high-degree polynomials is accurate, but expensive due time step restrictions, and results can be quite oscillatory

*We are pursuing two different approaches for advection that will work for large time steps on unstructured grids*

# 1. Extension of CSLAM[1] with Exact Cell Intersections

- In collaboration with I. Grindeanu (ANL)
- Semi-Lagrangian finite volume approach to advection
- Intersections for unstructured polygonal grids in spherical geometry from MOAB[2]



[1] Conservative Semi-Lagrangian Multi-tracer, Lauritzen, Nair, Ullrich JCP (2010)

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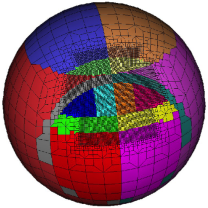

*Advantages*

- Allows for long time steps
- Tracer mass conserving and free stream preserving
- Geometric quantites are only computed once so cost is independent of number of tracers

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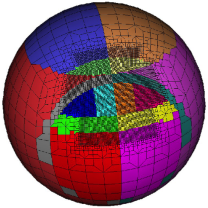

*Advantages*

- Allows for long time steps
- Tracer mass conserving and free stream preserving
- Geometric quantites are only computed once so cost is independent of number of tracers

*Disadvantages*

- Expensive to compute cell intersections
- Requires separate finite volume grid

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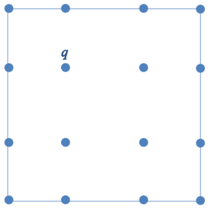
- Efficient, does not require geometric computations
- Fits naturally with native spectral element method used in CAM-SE

*Disadvantages*

- Requires optimization or other approach to ensure mass conservation

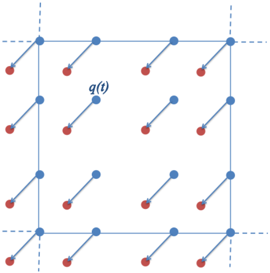
# Semi-Lagrangian Spectral Element Tracer Transport

- Consider a cell with tracer $q$ values at GLL nodes at time $t$



# Semi-Lagrangian Spectral Element Tracer Transport

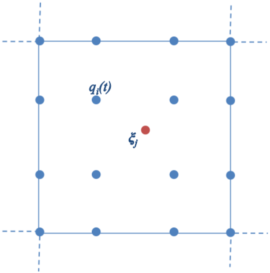
- Consider a cell with tracer $q$ values at GLL nodes at time $t$
- Compute backward Lagrangian trajectories of each node



# Semi-Lagrangian Spectral Element Tracer Transport

- Consider a cell with tracer $q$ values at GLL nodes at time $t$
- Compute backward Lagrangian trajectories of each node
- Locate Lagrangian points on Eulerian mesh $(\xi_1, \xi_2) = F^{-1}(\lambda, \theta)$
- Map Eulerian nodal values to Lagrangian nodes using spectral element basis

$$q_j^L(t) = \sum_{i=1}^{nNodes} q_i \phi_i(\xi_j^L)$$



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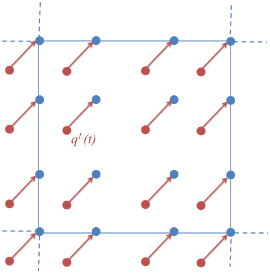
$$q_j^L(t) = \sum_{i=1}^{nNodes} q_i \phi_i(\xi_j^L)$$

- Lagrangian update of tracer values

$$q^{\mathsf{T}}(t + \Delta t) = q^L(t)$$



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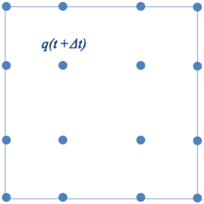
$$q_j^L(t) = \sum_{i=1}^{nNodes} q_i \phi_i(\xi_j^L)$$

- Lagrangian update of tracer values $q^{\mathsf{T}}(t + \Delta t) = q^L(t)$
- Perform optimization step



# Optimization

| Objective | Target | Constraints |
|---|---|---|
| $\lVert \widetilde{q} - q^T \rVert$<br>minimize the distance between the solution and a suitable target | $\partial_t q^{\mathsf{T}} + \mathbf{u} \cdot \nabla q^{\mathsf{T}} = 0$<br>stable and accurate solution, not required to possess all desired physical properties | $q^{min} \leq \widetilde{q} \leq q^{max}$<br>$\sum \widetilde{m}_i \widetilde{q}_i = Q$<br>desired physical properties viewed as constraints |

*Advantages*

- Solution is globally optimal with respect to the target and desired physical properties
- Decouples accuracy from enforcement of physical properties

# Optimization Algorithm[1]

$$\begin{cases} \text{minimize} \quad \frac{1}{2}\|\widetilde{q} - q^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \sum_{i=1}^{N} \widetilde{m}_i \widetilde{q}_i = Q, \quad q_i^{\min} \leq \widetilde{q} \leq q_i^{\max} \end{cases}$$

Lagrangian functional $\mathcal{L} : \mathbb{R}^N \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^N \to \mathbb{R}$

$$\mathcal{L}(\widetilde{q}, \lambda, \mu_1, \mu_2) = \frac{1}{2}\sum_{i=1}^{N}(\widetilde{q}_i - q_i^{\mathsf{T}})^2 - \lambda \sum_{i=1}^{N} \widetilde{q}_i -$$

$$\textstyle\sum_{i=1}^{N} \mu_{1,i} \left(\widetilde{q}_i - q_i^{min}\right) - \sum_{i=1}^{N} \mu_{2,i} \left(q_i^{max} - \widetilde{q}_i\right) \ ,$$

where $\widetilde{q} \in \mathbb{R}^N$ are the optimization variables, and $\lambda \in \mathbb{R}$, $\mu_1 \in \mathbb{R}^N$, and $\mu_2 \in \mathbb{R}^N$ are the Lagrange multipliers

[1] Based on the Optimization-Based Remap Algorithm (Bochev, Ridzal, Shashkov, JCP 2013)

# Optimization Algorithm[1]

$$\left\{\begin{array}{l} \text{minimize} \quad \frac{1}{2}\|\widetilde{q} - q^{\mathsf{T}}\|_{\ell_2}^2 \quad \text{subject to} \\ \sum_{i=1}^{N} \widetilde{m}_i \widetilde{q}_i = Q, \quad q_i^{\min} \le \widetilde{q} \le q_i^{\max} \end{array}\right.$$

Karush-Kuhn-Tucker (KKT) conditions:

$$\begin{aligned} \widetilde{q}_i = q_i^{\mathsf{T}} + \lambda + \mu_{1,i} - \mu_{2,i}; &\quad i = 1, \dots, N \\ q_i^{min} \le \widetilde{q}_i \le q_i^{max}; &\quad i = 1, \dots, N \\ \mu_{1,i} \ge 0\,, \quad \mu_{2,i} \ge 0; &\quad i = 1, \dots, N \\ \mu_{1,i}\left(\widetilde{q}_i - q_i^{min}\right) = 0\,, \quad \mu_{2,i}\left(-\widetilde{q}_i + q_i^{max}\right) = 0; &\quad i = 1, \dots, N \\ \textstyle\sum_{i=1}^{N} \widetilde{m}_i \widetilde{q}_i = Q & \end{aligned}$$

[1] Based on the Optimization-Based Remap Algorithm (Bochev, Ridzal, Shashkov, JCP 2013)

# Optimization Algorithm

For any *fixed* value of $\lambda$ a solution is given by

$$\begin{cases} \widetilde{q}_i = q_i^{\mathsf{T}} + \lambda; & \mu_{1,i} = \mu_{2,i} = 0 & \text{if} \quad q_i^{min} \le q_i^{\mathsf{T}} + \lambda \le q_i^{max} \\ \widetilde{q}_i = q_i^{min}; & \mu_{2,i} = 0,\ \mu_{1,i} = \widetilde{q}_i - q_i^{\mathsf{T}} - \lambda & \text{if} \quad q_i^{\mathsf{T}} + \lambda < q_i^{min} \\ \widetilde{q}_i = q_i^{max}; & \mu_{1,i} = 0,\ \mu_{2,i} = q_i^{\mathsf{T}} - \widetilde{q}_i + \lambda & \text{if} \quad q_i^{\mathsf{T}} + \lambda > q_i^{max}\,, \end{cases}$$

for all $i = 1, \ldots, N$.

Ignoring $\mu_1$ and $\mu_2$ and treating $\widetilde{q}_i$ as a function of $\lambda$ yields

$$\widetilde{q}_i(\lambda) = \text{median}(q_i^{min},\, q_i^{\mathsf{T}} + \lambda,\, q_i^{max})\,, \qquad i = 1, \ldots, N\,.$$

Adjust $\lambda$ in outer iteration to satisfy $\sum_{i=1}^{N} \widetilde{m}_i \widetilde{q}_i(\lambda) = Q$.

*The algorithm generally requires $\le 5$ outer secant iterations. In serial, it is as efficient as standard slope limiting or flux limiting techniques.*

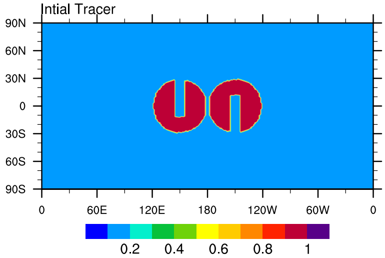
# Computational Examples

- Velocity fields
  - Solid body rotation
  - Nondivergent deformational flow field, $T = 5$

$$u(\lambda, \theta, t) = 2\sin^2(\lambda)\sin(2\theta)\cos(\pi t/T)$$

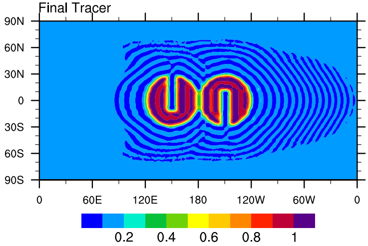
$$v(\lambda, \theta, t) = 2\sin(2\lambda)\cos(\theta)\cos(\pi t/T)$$

- Tracer distribution: notched cylinders centered at $(\lambda_1, \theta_1) = (5\pi/6, 0)$ and $(\lambda_2, \theta_2) = (7\pi/6, 0)$

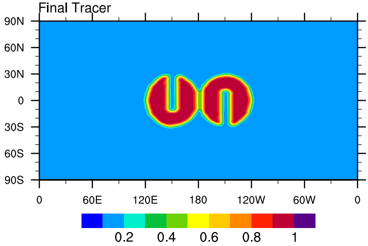


# Solid Body Rotation, 1.5° resolution

SE-SL




SE-SL Opt



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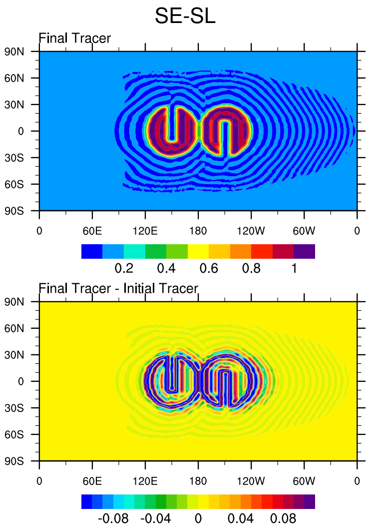

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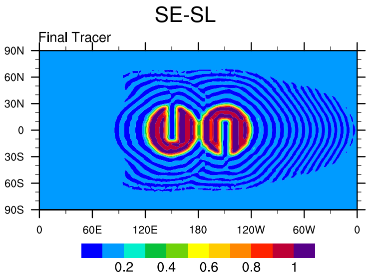
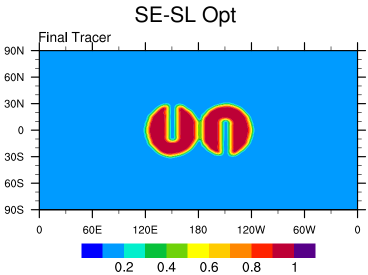


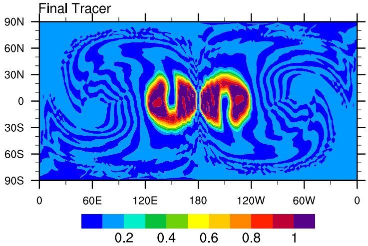

Mass error = -3.14e-3
Min value = -0.1223
Max value = 1.2472



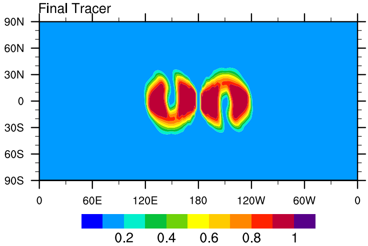

Mass error = 1.4e-13
Min value = 0.1
Max value = 1.0

# Deformational flow, 1.5° resolution

SE-SL




SE-SL Opt



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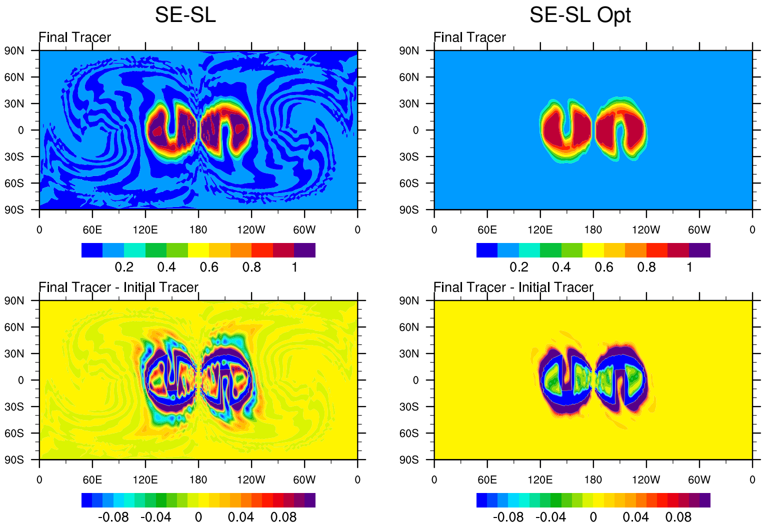

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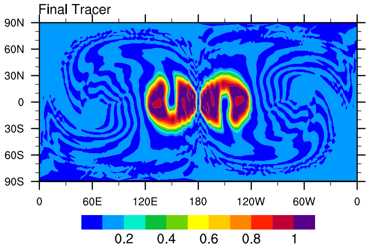
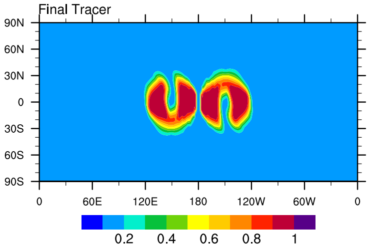
SE-SL




Mass error = -3.44e-3
Min value = -0.1070
Max value = 1.1934

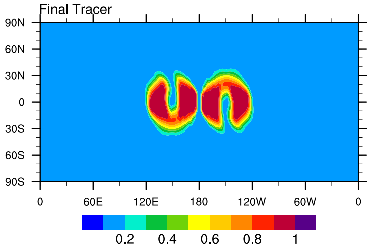
SE-SL Opt




Mass error = 1.69e-11
Min value = 0.1
Max value = 0.9979

# Open Questions

- How to define bounds for optimization? All DOFs in surrounding cells? Nearest neighbor DOFs?
- Can we modify the target to improve the final solution using smoothness indicators?
- How will the method scale on many processors? Will the global sum for each secant iteration be problematic?



# Conclusions

- Pursuing two approaches to tracer transport in CAM-SE
  - CSLAM-based algorithm using cell intersections computed with MOAB
  - Semi-Lagrangian spectral element (SL-SE) algorithm using optimization to enforce mass conservation
- SL-SE algorithm looks promising
  - Efficient, works for large time steps
  - Applicable to unstructured grids
  - Optimization algorithm succesfully conserves mass and enforces bounds
- Future Work
  - Complete implementation of new advection methods in HOMME/CAM-SE
  - Compare parallel efficiency and accuracy